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Registry Number:

255852-09-6

CA Index Name:

Uridine,

5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-2'-[[[(4,5-dimethoxy-2

-nitrophenyl)methoxy]carbonyl]amino]-, 3'-[2-cyanoethyl

bis(1-methylethyl)phosphoramidite] (9CI)

Formula:

C49 H57 N6 Q14 P

STN Files:

CAPLUS, CA, CASREACT

(Additional Information is available through STN International. Contact your information specialist, a local CAS representative, or the CAS Help Desk for

Assistance)

PROPERTY	VALUE	CONDITION	NOTE
H donors	2		ACD (1)
H acceptors	20	·	ACD (1)
Molecular Weight	984.98		ACD (1)
logP	9.877±0.950		ACD (1)
Freely Rotatable Bonds	25		ACD (1)
logD	6.78	pH 1	ACD (1)
logD	6.94	pH 4	ACD (1)
logD	9.30	pH 7	ACD (1)

# 282543-35-5P

15 October 2002

### SciFinder Scholar

Page: 2

Registry Number:

454464-20-1

**CA Index Name:** 

INDEX NAME NOT YET ASSIGNED

Formula:

C53 H62 Fe N5 O9 P

STN Files:

CAPLUS, CA, USPATFULL

(Additional Information is available through STN International. Contact your information specialist, a local CAS representative, or the CAS Help Desk for

Assistance)

Class Identifier:

Coordination Compound

#### ~1 Reference

## **Database**

REGISTRY (COPYRIGHT 2002 ACS)

Registry Number: 282543-35-5

CA Index Name: Uridine,

5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-2'-[[[7-(2,2-dimethyl-

1-oxopropoxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]-,

3'-[2-cyanoethyl bis(1-methylethyl)phosphoramidite] (9CI)

Formula: C54 H60 N5 O13 P

STN Files: CAPLUS, CA

PROPERTY	<u>VALUE</u>	CONDITION	NOTE
H donors	2		ACD (1)
H acceptors	18		ACD (1)
Molecular Weight	1018.05		ACD (1)
logP	9.527±0.889		ACD (1)
Freely Rotatable Bonds	23		ACD (1)
logD	6.43	pH 1	ACD (1)
logD	6.59	pH 4	ACD (1)
logD	8.95	pH 7	ACD (1)
logD	9.36	pH 8	ACD (1)
logD	8.19	pH 10	ACD (1)
рКа	8.81±0.40	Most Acidic	ACD (1)
pKa	7,44±0.50	Most Basic	ACD (1)
Molar Solubility	Sparingly Soluble	pH 1	ACD (1)

## SciFinder Scholar

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**Registry Number:** 

182005-99-8

**CA Index Name:** 

Thymidine,

5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-2'-[(trifluoroacetyl)ami

no]uridylylimino-(3'→5')-5'-deoxy- (9CI)

Formula:

C42 H44 F3 N6 O14 P

STN Files:

CAPLUS, CA

Absolute stereochemistry.

PROPERTY	VALUE	CONDITION	NOTE
H donors	6		ACD (1)
H acceptors	20		ACD (1)
Molecular Weight	944.80		ACD (1)
logP	2.627±1.081		ACD (1)
рКа	6.40±0.50	Most Basic	ACD (1)

#### Notes

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 (@ 1994-2002 ACD)

#### ~1 Reference

#### **Database**

REGISTRY (COPYRIGHT 2002 ACS)

Registry Number: 126139-47-7

CA Index Name: 2,4(1H,3H)-Pyrimidinedione,

1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-3-O-[[bis(1-methylethyl)amin o]methoxyphosphino]-2-deoxy-2-[[[(trifluoroacetyl)amino]acetyl]amino]-β-D

-arabinofuranosyl]- (9CI)

Formula: C41 H49 F3 N5 O10 P

STN Files: CAPLUS, CA, USPATFULL

(Additional Information is available through STN International. Contact your information specialist, a local CAS representative, or the CAS Help Desk for

Assistance)

PROPERTY	<u>VALUE</u>	CONDITION	NOTE
H donors	3		ACD (1)
H acceptors	15		ACD (1)
Molecular Weight	859.82		ACD (1)
logP	8.222±1.151		ACD (1)
Freely Rotatable Bonds	20		ACD (1)
logD	5.12	pH 1	ACD (1)
logD	5.18	pH 4	ACD (1)
logD	7.22	pH 7	ACD (1)
logD	7.88	pH 8	ACD (1)
logD	6.59	pH 10	ACD (1)
рКа	8.81±0.40	Most Acidic	ACD (1)

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Registry Number: 1

161016-72-4

**CA Index Name:** 

2,4(1H,3H)-Pyrimidinedione,

1-[2-deoxy-3-Q-(methylsulfonyl)-2-(4-morpholinyl)-5-Q-(triphenylmethy

I)-β-D-xylofuranosyl]- (9CI)

Formula:

C33 H35 N3 O8 S

**STN Files:** 

CAPLUS, CA, CASREACT

(Additional Information is available through STN International. Contact your information specialist, a local CAS representative, or the CAS Help Desk for

Assistance)

PROPERTY	VALUE	CONDITION	NOTE
H donors	1		ACD (1)
H acceptors	11		ACD (1)
Molecular Weight	633.71		ACD (1)
logP	4.521±0.648		ACD (1)
Freely Rotatable Bo	nds 10		ACD (1)
logD	1.63	pH 1	ACD (1)
logD	4.04	pH 4	ACD (1)
logD	4.51	pH 7	ACD (1)
logD	4.46	pH 8	ACD (1)
logD	3.31	pH 10	ACD (1)
рКа	8.81±0.40	Most Acidic	ACD (1)
pKa	4.30±0.20	Most Basic	ACD (1)
Molar Solubility	Sparingly Soluble	pH 1	ACD (1)
Molar Solubility	Sparingly Soluble	pH 4	ACD (1)
Molar Solubility	Sparingly Soluble	pH <b>7</b>	ACD (1)
Molar Solubility	Sparingly Soluble	pH 8	ACD (1)